KATHOLIEKE
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DEPARTEMENT TOEGEPASTE ECONOMISCHE WETENSCHAPPEN

RESEARCH REPORT 9945

OPTIMAL RESPONSE SURFACE DESIGNS IN THE PRESENCE OF RANDOM BLOCK EFFECTS

by

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D/1999/2376/45

Optimal Response Surface Designs in the Presence of Random Block Effects

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Abstract

The purpose of this paper is twofold. Firstly, it provides the reader with an overview of the literature on optimal response surface designs for random block effects models. Special attention is given to cases in which $\mathcal{D}$-optimal designs do not depend on the degree of correlation. These situations include some cases where the block size is greater than or equal to the number of model parameters, the case of minimum support designs and some orthogonally blocked designs. However, in many instances the optimal design depends on the degree of correlation and no exact optimal designs can be found in the literature. In the second part of this paper, an algorithm is presented that produces $\mathcal{D}$-optimal designs for these cases. Examples will illustrate the construction of optimal designs for each design problem described.

Keywords: design construction, $\mathcal{D}$-optimality, experimental design, correlated observations

1 Introduction

The theory of optimal designs for regression models usually assumes uncorrelated errors. However, there are many experimental situations in which this assumption is invalid because the experimental runs can not be carried out under homogeneous conditions. For example, the raw material used in a production process may be obtained in batches in which the quality can vary considerably from one batch to another. To account for this variation among the batches, a random batch effect should be added to the regression model. In the semi-conductor industry, it is of interest to investigate the effect of several factors on the resistance in computer chips. Here, measurements are taken using silicon wafers randomly drawn from a large lot. Therefore, the wafer effect should be considered as a random effect in the corresponding model. Chasalow (1992) describes an optometry experiment for exploring the dependence of corneal hydration control on the CO_2 level in a gaseous environment applied through a goggle covering a human subject's eyes. Since a response is measured for each eye, each human subject's pair of eyes provide a block of two possibly correlated observations. Other examples of experiments where there might be random block effects include agricultural experiments where multiple fields are used or chemistry experiments where runs are executed on different days or in different laboratories. The experimental design question in these examples is how to allocate the levels of the factors under investigation to the blocks. Although there exists an extensive literature on optimal block designs for treatment comparisons, optimal block designs for regression models have received much less attention. Atkinson and Donev (1989) and Cook and Nachtsheim (1989) propose an exchange algorithm for the computation of $\mathcal{D}$-optimal regression designs in the presence of fixed block effects. The derivation of approximate optimal regression designs in the presence of random block effects has been studied by Atkins (1994), Cheng (1995) and by Atkins and Cheng (1999). However, their approximate theory for the design of blocked experiments is of limited practical use in industrial environments where the number of blocks is typically small. Cheng (1995) as well as Atkins and Cheng (1999) also describe a special case in which the exact optimal design is easy to construct. Chasalow (1992) uses complete enumeration to find exact designs for quadratic regression when there are random block effects. For more complicated models, complete enumeration becomes impossible within a reasonable computing time. In this paper, we propose an exchange algorithm for this design problem. The analysis of response surface models with random block effects is discussed by Khuri (1992), who also derives general conditions for orthogonal blocking.

Assume that an experiment consists of n experimental runs arranged in b blocks of sizes $k_1, \ldots, k_b$ with $n = \sum_{i=1}^{b} k_i$. When the blocks are random, the model can be written as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma} + \boldsymbol{\varepsilon}, \tag{1}$$

where $\mathbf{y}$ is a vector of n observations on the response of interest, the vector $\boldsymbol{\beta} = [\beta_1, \ldots, \beta_p]'$ contains the p unknown fixed parameters, the vector $\boldsymbol{\gamma} = [\gamma_1, \ldots, \gamma_b]'$ contains the b random block effects and $\boldsymbol{\varepsilon}$ is a random error vector. The matrices $\mathbf{X}$ and $\mathbf{Z}$ are known and have dimension $n \times p$ and $n \times b$ respectively. $\mathbf{X}$ contains the polynomial expansions of the m factor levels at the n experimental runs. $\mathbf{Z}$ is of the form

$$\mathbf{Z} = \mathrm{diag}[\mathbf{1}_{k_1}, \ldots, \mathbf{1}_{k_b}], \tag{2}$$

where $\mathbf{1}_k$ is a $k \times 1$ vector of ones. It is assumed that $\mathrm{E}(\boldsymbol{\gamma}) = \mathbf{0}$, $\mathrm{E}(\boldsymbol{\varepsilon}) = \mathbf{0}$, $\mathrm{Cov}(\boldsymbol{\gamma}) = \sigma_\gamma^2 \mathbf{I}_b$, $\mathrm{Cov}(\boldsymbol{\varepsilon}) = \sigma_\varepsilon^2 \mathbf{I}_n$, and $\mathrm{Cov}(\boldsymbol{\gamma}, \boldsymbol{\varepsilon}) = \mathbf{0}$. The variance-covariance matrix of the observations $\mathrm{Cov}(\mathbf{y})$ can then be written as

$$\mathbf{V} = \sigma_\varepsilon^2 \mathbf{I}_n + \sigma_\gamma^2 \mathbf{Z}\mathbf{Z}'. \tag{3}$$

Suppose the entries of $\mathbf{y}$ are grouped per block, then

$$\mathbf{V} = \mathrm{diag}[\mathbf{V}_1, \ldots, \mathbf{V}_b], \tag{4}$$

where

$$\mathbf{V}_i = \sigma_\varepsilon^2(\mathbf{I}_{k_i} + \eta \mathbf{1}_{k_i}\mathbf{1}'_{k_i}), \tag{5}$$

and

$$\eta = \sigma_\gamma^2/\sigma_\varepsilon^2. \tag{6}$$

As a result, the error structure is compound symmetric. Observations within each block are correlated, whereas observations from different blocks are statistically independent. If the variance components are known, the best linear unbiased estimator (BLUE) of the unknown $\boldsymbol{\beta}$ is given by

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\mathbf{y}. \tag{7}$$

A design $\mathbf{X} = [\mathbf{X}'_1|\ldots|\mathbf{X}'_b]'$, where $\mathbf{X}_i$ is that part of $\mathbf{X}$ corresponding to the ith block, is called $\mathcal{D}$-optimal if it maximizes the determinant of the information matrix

$$\begin{aligned} \mathbf{M} &= \mathbf{X}'\mathbf{V}^{-1}\mathbf{X}, \\ &= \frac{1}{\sigma_\varepsilon^2}\sum_{i=1}^{b}\mathbf{X}'_i(\mathbf{I}_{k_i\times k_i} - \frac{\eta}{1+k_i\eta}\mathbf{1}_{k_i}\mathbf{1}'_{k_i})\mathbf{X}_i, \\ &= \frac{1}{\sigma_\varepsilon^2}\Big\{\mathbf{X}'\mathbf{X} - \sum_{i=1}^{b}\frac{\eta}{1+k_i\eta}(\mathbf{X}'_i\mathbf{1}_{k_i})(\mathbf{X}'_i\mathbf{1}_{k_i})'\Big\}. \end{aligned} \tag{8}$$

This expression shows that the optimal design depends on the degree of correlation η. When $\eta \to 0$, or equivalently $\sigma_\gamma^2 \to 0$, the design problem degenerates to the case of complete randomization in which the observations are uncorrelated. When $\eta \to \infty$, the design problem comes down to designing an experiment with fixed blocks (see Section 3.2). Finally, note that a model similar to (1) is used in Goos and Vandebroek (1999a, 1999b) to describe bi-randomization designs. The essential difference lies in the fact that the runs of a bi-randomization experiment are grouped in whole plots because they possess common factor levels for some of the experimental factors. In this paper, the grouping depends on a certain characteristic of the runs independent of the factors under investigation. In the optometry example, each pair of eyes is considered as a block because they belong to the same person.

In the next section, we consider three special cases in which the $\mathcal{D}$-optimal design does not depend on η. In Section 3, we establish a connection between the design of experiments in the presence of fixed block effects and the design of experiments in the presence of random block effects and we develop an efficient blocking algorithm to construct $\mathcal{D}$-optimal designs for model (1). Computational results are presented in Section 4.

2 Optimal designs that do not depend on η

In three specific cases, the $\mathcal{D}$-optimal design for model (1) does not depend on the variance ratio η. Firstly, we show that some specific orthogonally blocked designs are $\mathcal{D}$-optimal under random block effects. Atkins and Cheng (1999) as well as Cheng (1995) describe two other cases in which the optimal designs are independent of η. Atkins and Cheng (1999) show that exact optimal block designs can sometimes be constructed from the optimal approximate design for the uncorrelated model. This is possible only when the block size is greater than or equal to the number of model parameters. Cheng (1995) shows that the optimal minimum support designs can be obtained by combining an exact optimal design for the uncorrelated model with a balanced incomplete block design. In each case, the optimal block design is based on an optimal design for the uncorrelated model

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}, \tag{9}$$

where $\mathrm{Cov}(\boldsymbol{\varepsilon}) = \sigma_\varepsilon^2 \mathbf{I}_n$ and $\mathbf{y}$, $\mathbf{X}$ and $\boldsymbol{\beta}$ are defined as in the correlated model (1).

2.1 Orthogonally blocked designs

An orthogonal block design that is supported on the points of a $\mathcal{D}$-optimal design for the uncorrelated model (9) with

$$\mathbf{X}_i'\mathbf{1}_{k_i} = \mathbf{0}, \qquad (i = 1, \ldots, b), \tag{10}$$

is a $\mathcal{D}$-optimal design for model (1) if no intercept is included in the model. The design so obtained is optimal for any positive η, such that no prior knowledge of the variance components is needed. Note that the block size may be heterogeneous. It should also be pointed out that (10) can not always be fulfilled. For example, this is the case when the block size is an odd number and the optimal design for the uncorrelated model has factor levels -1 and +1 only.

Condition (10) is a special case of the general conditions for orthogonal blocking of response surface designs derived by Khuri (1992):

$$\mathbf{X}_i'\mathbf{1}_{k_i} = \frac{k_i}{n}\mathbf{X}'\mathbf{1}_n, \qquad (i = 1, \ldots, b). \tag{11}$$

Khuri (1992) shows that, under this condition, the generalized least squares estimator of $\boldsymbol{\beta}$ (see (7)) is equivalent to the estimator obtained by treating the block effects as fixed, but he does not address other design issues.

When (10) holds, the information matrix (8) simplifies to $\mathbf{X}'\mathbf{X}/\sigma_\varepsilon^2$, which is the information matrix on the unknown parameters in model (9). Moreover, we know from matrix algebra that $|\mathbf{A} - \mathbf{t}\mathbf{t}'| < |\mathbf{A}|$ for any vector $\mathbf{t} \neq \mathbf{0}$ and positive definite matrix $\mathbf{A}$. As a result, $|\mathbf{X}'\mathbf{X} - \mathbf{t}_i\mathbf{t}_i'| < |\mathbf{X}'\mathbf{X}|$ for $\mathbf{t}_i = \{\eta/(1+k_i\eta)\}^{1/2}(\mathbf{X}_i'\mathbf{1}_{k_i}) \neq \mathbf{0}$. The

Block 1			Block 2		
A	B	C	A	B	C
-1	-1	-1	+1	-1	-1
+1	+1	-1	-1	+1	-1
+1	-1	+1	-1	-1	+1
-1	+1	+1	+1	+1	+1

Table 1: Optimal block design for the whipped topping experiment.

matrix $\mathbf{X}'\mathbf{X} - \mathbf{t}_i\mathbf{t}_i'$ remains positive definite because it is still a variance-covariance matrix. Therefore, the above reasoning can be repeated for every $\mathbf{t}_i$ which allows us to conclude that

$$|\mathbf{X}'\mathbf{X}| > |\mathbf{X}'\mathbf{X} - \sum_{i=1}^{b} \frac{\eta}{1+k_i\eta}(\mathbf{X}_i'\mathbf{1}_{k_i})(\mathbf{X}_i'\mathbf{1}_{k_i})'|$$

when at least one $\mathbf{X}_i'\mathbf{1}_{k_i} \neq \mathbf{0}$. As a result, for a given $\mathbf{X}$, the $\mathcal{D}$-optimal design for model (1) has the observations assigned to the blocks such that (10) holds. Now, a $\mathcal{D}$-optimal design for the uncorrelated model (9) maximizes $|\mathbf{X}'\mathbf{X}/\sigma_\varepsilon^2|$. Therefore, arranging the n observations of a $\mathcal{D}$-optimal design for model (9) in blocks such that (10) holds is an optimal design strategy. When the model of interest contains an intercept, (10) changes into

$$\mathbf{X}_i'\mathbf{1}_{k_i} = \begin{pmatrix} k_i \\ \mathbf{0} \end{pmatrix}, \qquad (i = 1, \ldots, b), \tag{12}$$

provided that the first column of $\mathbf{X}$ corresponds to the intercept. This is shown in Appendix A. However, the conditions can be generalized because the $\mathcal{D}$-optimality criterion is invariant to a linear transformation of the factor levels. Therefore, any design for which (10) and (12) can be accomplished by applying a linear transformation on the factor levels is $\mathcal{D}$-optimal for the design problem considered here. Consider an experiment to optimize the stability of a whipped topping from Cook and Nachtsheim (1989) to illustrate how the results from this section allow us to construct a $\mathcal{D}$-optimal design in the presence of random block effects. The amount of two emusifiers (A and B) and the amount of fat (C) are expected to have an impact on the melting that occurs after the aerosol topping is dispensed. Suppose that the experimenters are interested in the linear effects and the two factor interactions only and that two laboratory assistants are available for eight observations. The familiar 2^3 factorial is a $\mathcal{D}$-optimal design with eight observations for estimating the effects of interest in the uncorrelated model. A $\mathcal{D}$-optimal design in the presence of random block effects is easily obtained by using ABC as the block generator. The resulting design is displayed in Table 1. It is easy to verify that condition (10) holds.

It is clear that conditions (10) and (12) can not be satisfied when quadratic terms are included in the model. The same goes for pure linear models and linear models with interactions when the block size is an odd number. This is because a $\mathcal{D}$-optimal design for the uncorrelated pure linear model or the linear model with interactions has factor levels -1 and +1 only.

2.2 Large block size

In some specific cases, a $\mathcal{D}$- and $\mathcal{A}$-optimal design for correlated model (1) can be constructed from the $\mathcal{D}$- and $\mathcal{A}$-optimal approximate design for the uncorrelated model (9) when the block size is larger than the number of model parameters.

Let $\{\mathbf{x}_1^*, \ldots, \mathbf{x}_h^*\}$ with weights $\{\mathbf{w}_1^*, \ldots, \mathbf{w}_h^*\}$ be a $\mathcal{D}$- or $\mathcal{A}$-optimal approximate design for the uncorrelated model (9). Atkins and Cheng (1999) prove that the $\mathcal{D}$- and $\mathcal{A}$-optimal design for model (1) with b blocks of size k consists of b identical blocks where each design point $\mathbf{x}_i$ is replicated kw_i times if kw_i is an integer for each i. The optimal design is then independent of η. This theorem is only valid when the model contains an intercept. It implicitly requires that the block size k is greater than or equal to the number of parameters p. As a matter of fact, each block consists of an optimal design for the uncorrelated model and has therefore at least size p.

This result has a serious impact on the design of this type of experiments. Firstly, no prior knowledge on η is required since the optimal design points only depend on model (9). Secondly, rather than using a computationally intensive blocking algorithm to generate a design with $n = bk$ observations, a k-point $\mathcal{D}$- or $\mathcal{A}$-optimal design for the uncorrelated model can be used in each block. Although occasions in which all kw_i are integer are rare, the result of Atkins and Cheng (1999) is expected to be useful when the block size k is large with respect to the number of parameters. In this case, the values kw_i can be rounded to the nearest integer without serious loss of design efficiency. Unfortunately, design problems for which $k \geq p$ seldomly occur in practice.

Well-known situations where all kw_i can be integer occur in mixture experiments and in the case of quadratic regresion on a single explanatory variable. In mixture experiments, the optimal approximate designs for first and second order models have equal weight on the s points of a simplex lattice design. $\mathcal{D}$-optimal block designs when k is a multiple of s consist of identical blocks in which the lattice design is replicated k/s times. The attentive reader will point out that mixture models typically do not contain an intercept and that Atkins and Cheng's theorem does not apply in that case. However, a linear transformation of the design matrix of a mixture experiment exists such that it does contain a column of ones. This is because the sum of the mixture components always equals one. For quadratic regression on one variable, the $\mathcal{D}$-optimal approximate design has weight $1/3$ on the points -1, 0 and 1. Therefore, a $\mathcal{D}$-optimal design for quadratic regression on $[-1, 1]$ in the presence of random block effects can be readily obtained when the block size is a multiple of three. Consider an experiment carried out to investigate the impact of the initial potassium/carbon (K/C) ratio on the desorption of carbon monoxide (CO) in the context of the gasification of coal. The experiment is described in Atkinson and Donev (1992). Let x and y denote the K/C ratio and the amount of CO desorbed respectively. Further, suppose four blocks of observations are available to the researcher and that the model of interest is given by

$$y = \beta_0 + \beta_1 x + \beta_2 x^2. \tag{13}$$

If the block size of the experiment is equal to three, a $\mathcal{D}$-optimal design with four blocks of three observations consists of four identical blocks in which -1, 0 and 1 each appear once. Similarly, a $\mathcal{D}$-optimal design with four blocks of six observations each consists of four identical blocks in which -1, 0 and 1 each appear twice. In a similar way, $\mathcal{A}$-optimal block designs for the coal gasification experiment can be constructed when the block size is a multiple of four. For example, an $\mathcal{A}$-optimal design with four blocks of eight observations has four identical blocks in which both -1 and 1 appear twice and 0 is replicated four times. This is because the $\mathcal{A}$-optimal approximate design for quadratic regression on $[-1, 1]$ has weight 1/4 on -1 and 1 and weight 1/2 on 0.

2.3 Minimum support designs

In this section, we restrict our attention to minimum support designs. A minimum support design for a model with p parameters is supported on exactly p distinct points $\mathbf{x}_1, \ldots, \mathbf{x}_p$. This class of designs is useful because experimenters are often reluctant to the copious use of different factor levels and design points. Using a smaller number of distinct points than p in the experiment would result in a singular information matrix. Cheng (1995) provides a method to construct $\mathcal{D}$-optimal minimum support designs for model (1) by combining a p-point $\mathcal{D}$-optimal design for the uncorrelated model (9) and a balanced incomplete block design (BIBD). BIBDs are a special case of balanced block designs (BBDs) and were originally meant for treatment comparisons. Shah and Sinha (1989) show that BIBDs are universally optimal for estimating treatment contrasts, i.e. they are $\mathcal{A}$-, $\mathcal{D}$- and $\mathcal{E}$-optimal as well as optimal with respect to any generalized optimality criterion. They also show that this property remains valid for any positive η when observations within the same block of the BIBD have a compound symmetric correlation structure. An instructive introduction on BIBDs can be found in Cox (1958). BIBDs have the following properties:

1. each block contains the same number of observations,
2. each treatment occurs the same number of times in the entire experiment,
3. the number of times two different treatments occur together in a block is equal for all pairs of treatments.

Suppose $\{\mathbf{x}_1, \ldots, \mathbf{x}_p\}$ is a $\mathcal{D}$-optimal design with p observations for the uncorrelated model (9) and that a BIBD exists with p treatments and b blocks of size k, then using the p design points as treatments in the BIBD yields a design that is $\mathcal{D}$-optimal in the class of block designs with p points and b blocks of size k. Like in Sections 2.1 and 2.2, no prior knowledge on η is required and only a small design for the uncorrelated model has to be computed. The main drawback of this approach is that no BIBD can be found for certain combinations of block sizes and numbers of treatments.

As an illustration, consider a modified version of the constrained mixture experiment for estimating the impact of three factors on the electric resistivity of a modified acrylonitrile powder described in Atkinson and Donev (1992). The factors under investigation are

x_1 copper sulphate ($CuSO_4$),
x_2 sodium thiosulphate ($Na_2S_2O_3$),
x_3 glyoxal $(CHO)_2$.

The following constraints were imposed on the factor levels:

$$\begin{array}{ccccc} 0.2 & \leq & x_1 & \leq & 0.8, \\ 0.2 & \leq & x_2 & \leq & 0.8, \\ 0.0 & \leq & x_3 & \leq & 0.6. \end{array}$$

Assume that the model is given by the second-order Scheffé polynomial

$$y = \sum_{i=1}^{3} \beta_i x_i + \sum_{i=1}^{2} \sum_{j=i+1}^{3} \beta_{ij} x_i x_j. \tag{14}$$

A $\mathcal{D}$-optimal design with six observations for this model is given by the second-order simplex lattice design on the constrained design region. This is illustrated in Figure 1. Now, suppose that 10 experimenters are available and that 30 observations are considered desirable. Combining the $\mathcal{D}$-optimal design in Figure 1 and a BIBD for 6 treatments and 10 blocks of size 3 then yields an optimal design in the class of minimum support designs. The BIBD is shown in Table 2. The experiment is carried out by using each of the six design points as a treatment in the BIBD. Note that the blocks and the treatments are written in lexicographic order and should be randomized before conducting the experiment.

3 Optimal designs: the general case

As was already mentioned, the results on orthogonally blocked experiments of Section 2.1 can only be used for pure linear models or linear models with interactions when the block size is an even number. Similarly, the approach from Section 2.2

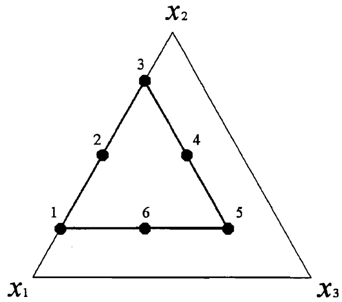


Figure 1: $\mathcal{D}$-optimal design for the constrained mixture experiment.

Block	Treatments	Block	Treatments
1	1 2 5	6	2 3 4
2	1 2 6	7	2 3 5
3	1 3 4	8	2 4 6
4	1 3 6	9	3 5 6
5	1 4 5	10	4 5 6

Table 2: BIBD with 6 treatments and 10 blocks of size 3.

requires a large and homogeneous block size. Even then, it can only be used in a limited number of cases. Finally, the theoretical result on minimum support designs in Section 2.3 can not be used when no suitable BIBD exists or when the number of support points is allowed to be larger than the number of unknown parameters. As a result, many experimental situations exist where the optimal design depends on the degree of correlation η.

In this section, we will first review the recent work on the topic of designing experiments under random blocks. Next, it will be shown that the design problem at hand is related to that considered in Atkinson and Donev (1989) and Cook and Nachtsheim (1989). We also present a point exchange algorithm to compute exact response surface designs in the presence of random block effects. In Section 4, some computational results are discussed.

3.1 Literature review

The general design problem for response surface models with random block effects has received attention in Chasalow (1992), Atkins (1994), Cheng (1995) and Atkins and Cheng (1999). Chasalow (1992) presents a complete enumeration approach to find exact optimal designs and applies it to the case of quadratic regression on $[-1, 1]$. This approach involves enumerating all possible blocks of the appropriate size as well as all possible designs consisting of these blocks. Therefore, it is computationally intensive when more than one factor is under investigation. Suppose that an experiment with 6 blocks of 4 observations is conducted to estimate a full quadratic model in 2 variables with 3 factor levels. Since we have $3^2 = 9$ factor level combinations, the number of different blocks of 4 observations is given by

$$\binom{4+9-1}{4} = 495.$$

As a result, the total number of designs considered is given by

$$\binom{6+495-1}{6} \sim 10^{13}.$$

It is clear that increasing the number of experimental variables or the number of factor levels would further complicate the search for an optimal design. Cheng (1995) and Atkins and Cheng (1999) use an approximate theory to compute $\mathcal{D}$-optimal designs for quadratic regression on $[-1, 1]$. They point out that the weights of the different blocks as well as the factor levels in the $\mathcal{D}$-optimal design depend on η. For instance, Cheng (1995) shows that the approximate $\mathcal{D}$-optimal design with blocks of size two is supported on the blocks $(1; -a_\eta)$, $(-1; a_\eta)$ and $(-1; 1)$ $(a_\eta \geq 0)$ with weights $\varepsilon_\eta/2$, $\varepsilon_\eta/2$ and $1 - \varepsilon_\eta$ respectively. For example, for $\eta = 0.25$ the optimal values for a_η and ε_η amount to 0.059255 and 0.675536 respectively. Cheng (1995) shows that $a_\eta \to 0$ and $\varepsilon_\eta \to 2/3$ when η approaches zero. Atkins (1994) uses the same approximate theory to compute $\mathcal{D}$-optimal designs for general design problems in the presence of random block effects. Although these approximate designs provide useful insights, they are often of little use in practice, especially when the number of blocks is small.

Apart from Atkins (1994), the focus has been on designs for quadratic regression. In addition, most work has concentrated on approximate designs rather than exact designs. In the sequel of this paper, only exact designs will be considered.

3.2 Fixed block effects

If fixed block effects are assumed instead of random block effects, the model can be rewritten as

$$\begin{aligned} \mathrm{y} &= \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\alpha} + \boldsymbol{\varepsilon}, \\ &= \mathbf{W}\boldsymbol{\tau} + \boldsymbol{\varepsilon}, \end{aligned} \tag{15}$$

where $\mathbf{W} = [\mathbf{X} \quad \mathbf{Z}]$, $\boldsymbol{\tau} = [\boldsymbol{\beta}' \quad \boldsymbol{\alpha}']'$ and $\mathrm{E}(\boldsymbol{\varepsilon}) = \mathbf{0}$ and $\mathrm{Cov}(\boldsymbol{\varepsilon}) = \sigma_\varepsilon^2\mathbf{I}$. Algorithms to construct $\mathcal{D}$-optimal blocking designs for this model have been proposed by Atkinson and Donev (1989) and by Cook and Nachtsheim (1989). Under model (15), the $\mathcal{D}$-optimal design for estimating $\boldsymbol{\tau}$ is equivalent to the $\mathcal{D}_\beta$-optimal design, i.e. the $\mathcal{D}$-optimal design for model (15) when interest is in estimating $\boldsymbol{\beta}$ only. In other words, maximizing $|\mathbf{W}'\mathbf{W}|$ and $|\mathbf{X}'\{\mathbf{I}-\mathbf{Z}(\mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}'\}\mathbf{X}|$ turns out to be equivalent. In Appendix B, it is shown that the latter determinant can be written as

$$|\mathbf{X}'\mathbf{X}-\sum_{i=1}^{b}\frac{1}{k_i}(\mathbf{X}_i'\mathbf{1}_{k_i})(\mathbf{X}_i'\mathbf{1}_{k_i})'|. \tag{16}$$

The matrix in (16) can be obtained from (8) when $\eta \to \infty$. For this reason, the $\mathcal{D}$-optimal designs for model (15) with fixed blocks and model (1) with random blocks will be equivalent for large η. Another consequence is that the designs derived in Section 2 are $\mathcal{D}$-optimal as well when the block effects are fixed instead of random.

Blocked experiments that are generated for fixed block effects models can be used when the blocks are random as well. We have shown that this makes sense if η is large. However, it is expected that these designs will not be optimal for practical values of η. The algorithms also fail to produce designs when $p+b>n$. This is because b block effects need to be estimated when the blocks are fixed rather than random. For these reasons, we have developed an algorithm to compute $\mathcal{D}$-optimal designs in the presence of random block effects. Designs can be produced as soon as $n \geq p$.

3.3 Generic point exchange algorithm

Unlike Chasalow (1992), we have chosen to use a point exchange algorithm to compute $\mathcal{D}$-optimal designs under random block effects. This is because enumerating all possible blocks and designs is a hopeless task when two or more factors are under investigation and when more than three factor levels are considered. Point exchange algorithms have been used for a variety of design problems, one of them being the blocking of response surface designs when the block effects are fixed. This topic is treated in Atkinson and Donev (1989) and Cook and Nachtsheim (1989). The algorithm of Atkinson and Donev (1989) first computes a n-point starting design which is then improved by substituting a design point with a point from the list of candidate points until no further improvement in $\mathcal{D}$-efficiency can be made. The starting design is partly generated in a random fashion and completed by a greedy heuristic. In order to avoid being stuck in a locally optimal design, more than one starting design is generated and the exchange procedure is repeated. Each repetition of these steps is called a try. In contrast, Cook and Nachtsheim (1989) only use one try. In order to obtain a starting design, they compute a p-point design for model (9) and use these points to compose a nonsingular blocking design. Like in Atkinson and Donev (1989), the starting design is improved by exchanging design points with candidate points. The resulting design is further improved by interchanging observations from different blocks.

In the generic algorithm described here, more than one try is used and the starting designs are partly composed in a random fashion and completed by sequentially adding the candidate point with the largest prediction variance. In order to improve the initial design, both exchanging design points with candidate points and interchanging observations from different blocks are considered. The input to the algorithm consists of the number of observations n, the number of blocks b, the block sizes k_i $(i = 1, \dots, b)$, the number of model parameters p, the order of the model, the number of explanatory variables m and the structure of their polynomial expansion. In addition, an estimate of η must be provided. A reasonable guess is usually satisfactory because the optimal block designs turn out to be optimal for a wide range of η-values. Typically, information on η is available from prior experiments of a similar kind. Khuri (1992) analyzes an experiment in which the effect of temperature and time on shear strength is investigated and obtains $\hat{\eta} = 0.2928$. The blocks were the batches of experimental material randomly selected from the warehouse supply. Further details on the algorithm are given in Appendix C. It was implemented in Fortran 77 and is available from the authors.

4 Computational results

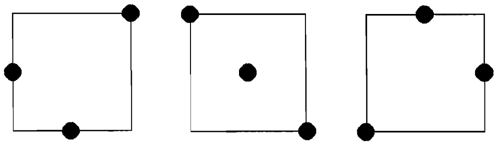
We have generated $\mathcal{D}$-optimal block designs for various combinations of the number of observations n, the number of blocks b and the number of experimental variables m. It turns out that taking into account the compound symmetric error structure is especially useful when the number of experimental variables exceeds two and when the model is not pure linear. When $n > p + b$, we were able to compare the random block designs generated by the algorithm from the previous section to the fixed block designs generated by the algorithms of Atkinson and Donev (1989) and Cook and Nachtsheim (1989). Design points were chosen from the 3^m factorial design.

Consider the 9-point $\mathcal{D}$-optimal design with three blocks of size three. The optimal designs for $\eta \leq 3.8790$ and $\eta \geq 3.8790$ are displayed in Figure 2a and 2b respectively and are denoted by RBD and FBD respectively. The design for $\eta \geq 3.8790$ coincides with the $\mathcal{D}$-optimal fixed block design. An interesting feature of the design for small η is that its projection, obtained by ignoring the blocks, results in the 3^2 factorial, which is the $\mathcal{D}$-optimal design for the uncorrelated model (9). For the design in Figure 2b, this is not the case.

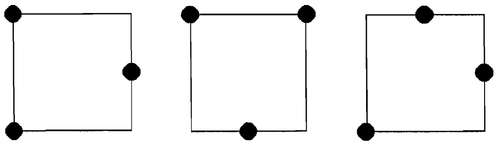
In order to compare the $\mathcal{D}$-criterion values of random block designs and fixed block designs under different degrees of correlation, we have computed the relative $\mathcal{D}$-efficiencies

$$\frac{|\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}|}{|\mathbf{A}'\mathbf{V}^{-1}\mathbf{A}|}, \tag{17}$$

where $\mathbf{X}$ is the design matrix of the random block design under consideration and $\mathbf{A}$ is the design matrix of the fixed block design for the same design problem. In Figure 3, the relative efficiency of the random block design in Figure 2a with respect



(a) $\eta \leq 3.8790$ (RBD)



(b) $\eta \geq 3.8790$ (FBD)

Figure 2: $\mathcal{D}$-optimal design with 3 blocks of size 3 for the full quadratic model in 2 variables.

to the fixed block design in Figure 2b is displayed. It is clear that RBD outperforms FBD for any practical value of η. For η close to zero, the former is 20% more efficient than the latter. However, the efficiency gain obtained by taking into account the correlation in the design phase decreases as the degree of correlation increases. For $\eta \geq 3.8790$, FBD is better than RBD. This is consistent with the fact that the optimal random block design for large η is equal to the optimal fixed block design.

The picture for more complicated models looks somewhat different. Consider for example a full quadratic model in four variables and suppose six blocks of four observations are available for experimentation. For this design problem, we have found one random block design that is optimal for $\eta \leq 0.00108$ and one that is optimal for $0.00108 \leq \eta \leq 2685048.042$. Let these designs be denoted by RBD1 and RBD2 respectively. The projection of RBD1 obtained by ignoring the blocks yields the $\mathcal{D}$-optimal designs for the uncorrelated full quadratic model in four variables, while the projection of RBD2 is nearly $\mathcal{D}$-optimal. The projection of the fixed block design for this design problem (FBD) is not even close to $\mathcal{D}$-optimal for the uncorrelated model. Both RBD1 and RBD2 are compared to the fixed block design FBD for the same design problem in Figure 4. For $\eta \leq 0.12269$, RBD1 is better than FBD. However, FBD is outperformed by RBD2 for any practical value of η. Compared to FBD, the $\mathcal{D}$-criterion value is increased by more than 20% for small degrees of correlation and by more than 50% when the degree of correlation exceeds unity.

We obtained similar results for both first and second order models for other combinations of n, b and k. In general, we can conclude that $\mathcal{D}$-optimal designs in the presence of random block effects fundamentally differ from $\mathcal{D}$-optimal designs in the

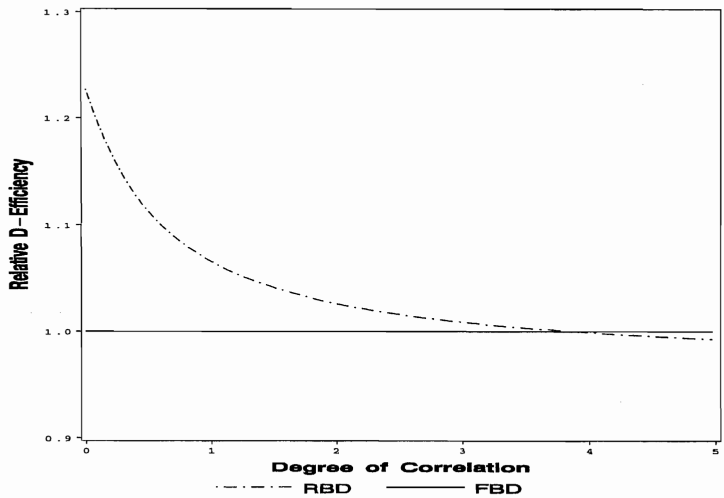


Figure 3: Comparison of the $\mathcal{D}$-efficiency of the designs in Figure 2 for the full quadratic model in 2 variables.

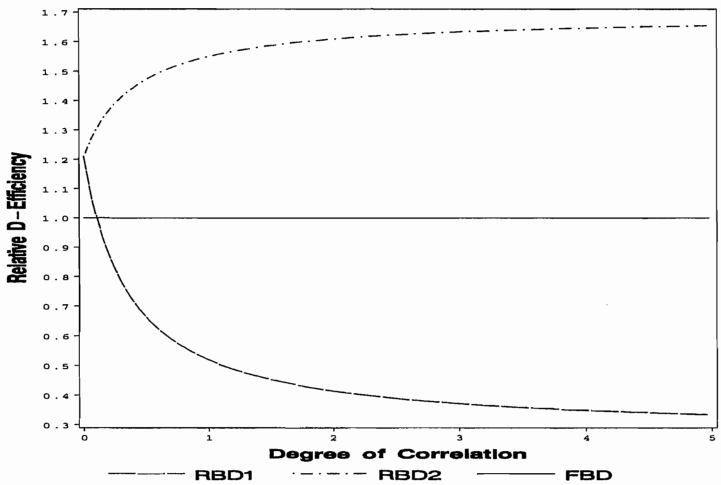


Figure 4: Comparison of the $\mathcal{D}$-efficiency of the random block designs RBD1 and RBD2 to the fixed block design FBD with 6 blocks of 4 observations for the full quadratic model in 4 variables.

presence of fixed block effects. While the projection of the random block designs is in many cases $\mathcal{D}$-optimal for the uncorrelated model, this is not at all true for the projection of the fixed block design. Therefore, the construction of the random block designs can be seen as assigning observations of a highly efficient design for the uncorrelated model to blocks in order to obtain an efficient design for the correlated model. On the contrary, an efficient design in the presence of fixed block effects is obtained from an inefficient design for the uncorrelated model. Computational results also indicate that the random block designs are highly robust to misspecification of η. Typically, only one, two or three different random block designs were found for a given design problem. As a result, these designs are optimal for wide ranges of η. Precise prior knowledge of the degree of correlation η is therefore not needed to generate $\mathcal{D}$-optimal random block designs. It should be pointed out that sometimes, unlike the example given in Figure 2, the fixed block design turns out to be the optimal random block design as well for models with one and two experimental variables even for relatively small η. For models with more than two variables, the fixed block design and the optimal random block design only coincide when observations within the same block are nearly perfectly correlated, that is for very large η.

In this section, we have shown that $\mathcal{D}$-optimal response surface designs in the presence of random block effects substantially differ from $\mathcal{D}$-optimal response surface designs in the presence of fixed block effects. In addition, they are highly insensitive to the degree of correlation which is very important from a practical point of view.

5 Conclusion

In this paper, we have concentrated on the computation and the features of exact optimal response surface designs in the presence of random block effects. Although approximate designs under random block effects have received attention by several authors, exact designs have been considered only by Chasalow (1992). His approach of complete enumeration is however computationally prohibitive. Therefore, we have developed a point exchange algorithm to compute optimal random block designs. These designs substantially differ from blocked experiments designed for models with fixed block effects. In addition, they are shown to be optimal for wide ranges of the degree of correlation. This implies that precise prior knowledge is not required to compute $\mathcal{D}$-optimal designs in the presence of random block effects. In the paper, it is also shown that some specific orthogonally blocked designs are optimal for any degree of correlation η. Two other cases in which the optimal design does not depend on η are described as well. Examples were given to illustrate the theoretical results.

Acknowledgement

Peter Goos is supported by a doctoral research grant from the Fund for Scientific Research – Flanders (Belgium).

Appendix A

Let $\boldsymbol{\beta} = [\beta_0 \quad \tilde{\boldsymbol{\beta}}']'$ and $\mathbf{X} = [\mathbf{1}_n \quad \tilde{\mathbf{X}}]$ and rewrite model (1) as

$$\mathbf{y} = \beta_0 \mathbf{1}_n + \tilde{\mathbf{X}}\tilde{\boldsymbol{\beta}} + \mathbf{Z}\boldsymbol{\gamma} + \boldsymbol{\varepsilon}, \tag{A1}$$

where β_0 is the intercept and $\tilde{\boldsymbol{\beta}}$ and $\tilde{\mathbf{X}}$ are the parts of $\boldsymbol{\beta}$ and $\mathbf{X}$ not corresponding to the intercept. Condition (12) then simplifies to

$$\tilde{\mathbf{X}}_i'\mathbf{1}_{k_i} = \mathbf{0}, \qquad (i = 1, \ldots, b). \tag{A2}$$

The information matrix on $\boldsymbol{\beta}$ is given by

$$\mathbf{X}'\mathbf{V}^{-1}\mathbf{X} = \begin{bmatrix} \mathbf{1}_n'\mathbf{V}^{-1}\mathbf{1}_n & \mathbf{1}_n'\mathbf{V}^{-1}\tilde{\mathbf{X}} \\ \tilde{\mathbf{X}}'\mathbf{V}^{-1}\mathbf{1}_n & \tilde{\mathbf{X}}'\mathbf{V}^{-1}\tilde{\mathbf{X}} \end{bmatrix}.$$

The $\mathcal{D}$-optimal design therefore maximizes

$$|\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}| = (\mathbf{1}_n'\mathbf{V}^{-1}\mathbf{1}_n)|\tilde{\mathbf{X}}'\mathbf{V}^{-1}\tilde{\mathbf{X}} - \tilde{\mathbf{X}}'\mathbf{V}^{-1}\mathbf{1}_n(\mathbf{1}_n'\mathbf{V}^{-1}\mathbf{1}_n)^{-1}\mathbf{1}_n'\mathbf{V}^{-1}\tilde{\mathbf{X}}|.$$

Since $c_1 = \mathbf{1}_n'\mathbf{V}^{-1}\mathbf{1}_n = \sigma_\varepsilon^{-2}\sum_{i=1}^{b} k_i/(1+k_i\eta)$ is constant over all possible designs, the optimal design only depends on

$$\tilde{\mathbf{X}}'\mathbf{V}^{-1}\tilde{\mathbf{X}} - \tilde{\mathbf{X}}'\mathbf{V}^{-1}\mathbf{1}_n(\mathbf{1}_n'\mathbf{V}^{-1}\mathbf{1}_n)^{-1}\mathbf{1}_n'\mathbf{V}^{-1}\tilde{\mathbf{X}}. \tag{A3}$$

Letting $c_{2i} = 1/(1+k_i\eta)$ for $i = 1, \ldots, b$ and substituting

$$\tilde{\mathbf{X}}'\mathbf{V}^{-1}\tilde{\mathbf{X}} = \sigma_\varepsilon^{-2}\Big\{\tilde{\mathbf{X}}'\tilde{\mathbf{X}} - \sum_{i=1}^{b}\frac{\eta}{1+k_i\eta}(\tilde{\mathbf{X}}_i'\mathbf{1}_{k_i})(\tilde{\mathbf{X}}_i'\mathbf{1}_{k_i})'\Big\},$$

and

$$\begin{aligned}
\tilde{\mathbf{X}}'\mathbf{V}^{-1}\mathbf{1}_n &= \sum_{i=1}^{b}\tilde{\mathbf{X}}_i'\mathbf{V}_i^{-1}\mathbf{1}_{k_i}, \\
&= \sigma_\varepsilon^{-2}\sum_{i=1}^{b}(\tilde{\mathbf{X}}_i'\mathbf{1}_{k_i} - \frac{\eta}{1+k_i\eta}\tilde{\mathbf{X}}_i'\mathbf{1}_{k_i}\mathbf{1}_{k_i}'\mathbf{1}_{k_i}), \\
&= \sigma_\varepsilon^{-2}\sum_{i=1}^{b}(\tilde{\mathbf{X}}_i'\mathbf{1}_{k_i} - \frac{k_i\eta}{1+k_i\eta}\tilde{\mathbf{X}}_i'\mathbf{1}_{k_i}), \\
&= \sigma_\varepsilon^{-2}\sum_{i=1}^{b}\frac{\tilde{\mathbf{X}}_i'\mathbf{1}_{k_i}}{1+k_i\eta}, \\
&= \sigma_\varepsilon^{-2}\sum_{i=1}^{b}c_{2i}\tilde{\mathbf{X}}_i'\mathbf{1}_{k_i},
\end{aligned}$$

in (A3) yields

$$\tilde{\mathbf{X}}'\tilde{\mathbf{X}} - \sum_{i=1}^{b} \frac{\eta}{1+k_i\eta}(\tilde{\mathbf{X}}_i'\mathbf{1}_{k_i})(\tilde{\mathbf{X}}_i'\mathbf{1}_{k_i})' - c_1^{-1}\sigma_\varepsilon^{-2}(\sum_{i=1}^{b} c_{2i}\tilde{\mathbf{X}}_i'\mathbf{1}_{k_i})(\sum_{i=1}^{b} c_{2i}\tilde{\mathbf{X}}_i'\mathbf{1}_{k_i})', \tag{A4}$$

apart from the constant σ_ε^{-2}. Since $|\mathbf{A} - \mathbf{t}\mathbf{t}'| < |\mathbf{A}|$ for any positive definite matrix $\mathbf{A}$ and vector $\mathbf{t} \neq \mathbf{0}$, assigning observations to the blocks such that (10) holds is the optimal strategy for a given $\tilde{\mathbf{X}}$. A $\mathcal{D}$-optimal design for the uncorrelated model (9) maximizes

$$\begin{aligned}|\mathbf{X}'\mathbf{X}| &= (\mathbf{1}_n'\mathbf{1}_n)|\tilde{\mathbf{X}}'\tilde{\mathbf{X}} - \tilde{\mathbf{X}}'\mathbf{1}_n(\mathbf{1}_n'\mathbf{1}_n)^{-1}\mathbf{1}_n'\tilde{\mathbf{X}}| \\ &= n|\tilde{\mathbf{X}}'\tilde{\mathbf{X}} - n^{-1}(\tilde{\mathbf{X}}'\mathbf{1}_n)(\tilde{\mathbf{X}}'\mathbf{1}_n)'|,\end{aligned}$$

which simplifies to $n|\tilde{\mathbf{X}}'\tilde{\mathbf{X}}|$ when (A2) holds. Therefore, an orthogonal design that is supported on the $n = \sum_{i=1}^{b} k_i$ points of a $\mathcal{D}$-optimal design for the uncorrelated model (9) such that (A2), or equivalently (12), holds, is a $\mathcal{D}$-optimal design for model (1).

Appendix B

Assume that the rows in $\mathbf{X}$ and $\mathbf{Z}$ are grouped per block and that the corresponding part of the design matrix is denoted by $\mathbf{X}_i$. The information matrix on $\boldsymbol{\beta}$ under model (15) is given by

$$\mathbf{X}'\{\mathbf{I} - \mathbf{Z}(\mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}'\}\mathbf{X} = \mathbf{X}'\mathbf{X} - \mathbf{X}'\mathbf{Z}(\mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}'\mathbf{X}. \tag{A5}$$

Since $\mathbf{Z}'\mathbf{Z} = \mathrm{diag}(k_1, \ldots, k_b)$ and thus $(\mathbf{Z}'\mathbf{Z})^{-1} = \mathrm{diag}[k_1^{-1}, \ldots, k_b^{-1}]$, we have that

$$\mathbf{Z}(\mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}' = \mathrm{diag}[k_1^{-1}(\mathbf{1}_{k_1}\mathbf{1}_{k_1}'), \ldots, k_b^{-1}(\mathbf{1}_{k_b}\mathbf{1}_{k_b}')]. \tag{A6}$$

Expression (A5) then becomes

$$\mathbf{X}'\mathbf{X} - \sum_{i=1}^{b} \frac{1}{k_i}(\mathbf{X}_i'\mathbf{1}_{k_i})(\mathbf{X}_i'\mathbf{1}_{k_i})'.$$

Appendix C

We denote the set of g candidate points by G, the set of b blocks by B, the set of k_i not necessarily distinct design points belonging to the $i$the block of a given design D by D_i ($i = 1, \ldots, b$) and the $\mathcal{D}$-criterion value of a given design D by $\mathcal{D}$. The best design found at a given time by the algorithm will denoted by D^*. Its blocks will be denoted by D_i^* ($i = 1, \ldots, b$) and the corresponding $\mathcal{D}$-criterion value by $\mathcal{D}^*$. For simplicity, we denote the information matrix of the experiment by $\mathbf{M}$.

The singularity while constructing a starting design is overcome by using $\mathbf{M} + r\mathbf{I}$ instead of $\mathbf{M}$ with r a small positive number. Finally, we denote the number of tries by t and the number of the current try by t_c. The algorithm starts by specifying the set of grid points $G = \{1, \ldots, g\}$ and proceeds as follows:

1. Set $\mathcal{D}^* = 0$ and $t_c = 1$.
2. Set $\mathbf{M} = r\mathbf{I}$ and $D_i = \emptyset$ $(i = 1, \ldots, b)$.
3. Generate starting design.
   (a) Randomly choose m $(1 \leq m \leq p)$.
   (b) Do m times:
      i. Randomly choose $i \in G$.
      ii. Randomly choose $j \in B$.
      iii. If $\#D_j < k_j$, then $D_j = D_j \cup \{i\}$, else go to step ii.
      iv. Update $\mathbf{M}$.
   (c) Do $n - m$ times:
      i. Determine $i \in G$ with largest prediction variance.
      ii. Randomly choose $j \in B$.
      iii. If $\#D_j < k_j$, then $D_j = D_j \cup \{i\}$, else go to step ii.
      iv. Update $\mathbf{M}$.
4. Compute $\mathbf{M}$ and $\mathcal{D}$. If $\mathcal{D} = 0$, then go to step 2, else continue.
5. Evaluate exchanges.
   (a) Set $\delta = 1$.
   (b) $\forall i \in B, \forall j \in D_i, \forall k \in G, j \neq k$:
      i. Compute the effect $\delta_{ij}^k = \mathcal{D}'/\mathcal{D}$ of exchanging j by k in the ith block.
      ii. If $\delta_{ij}^k > \delta$, then $\delta = \delta_{ij}^k$ and store i, j and k.
6. If $\delta > 1$, then go to step 7, else go to step 8.
7. Carry out best exchange.
   (a) $D_i = D_i \backslash \{j\} \cup \{k\}$.
   (b) Update $\mathbf{M}$ and $\mathcal{D}$.
8. Evaluate interchanges.
   (a) Set $\delta = 1$.
   (b) $\forall i, j \in B, i < j, \forall k \in D_i, \forall l \in D_j, k \neq l$:
      i. Compute the effect $\delta_{ik}^{jl} = \mathcal{D}'/\mathcal{D}$ of moving k from block i to j and l from block j to i.

ii. If $\delta_{ik}^{jl} > \delta$, then $\delta = \delta_{ik}^{jl}$ and store i, j, k and l.

9. If $\delta > 1$, then go to step 10, else go to step 11.

10. Carry out best interchange.

    (a) $D_i = D_i \backslash \{k\} \cup \{l\}$.

    (b) $D_j = D_j \backslash \{l\} \cup \{k\}$.

    (c) Update $\mathbf{M}$ and $\mathcal{D}$.

11. If $\mathcal{D} > \mathcal{D}^*$, then $\mathcal{D}^* = \mathcal{D}$, $\forall i \in B : D_i^* = D_i$.

12. If $t_c < t$, then $t_c = t_c + 1$ and go to step 2, else stop.

Like in the BLKL algorithm of Atkinson and Donev (1989), the algorithm allows for the possibility to consider only grid points with a large prediction variance for inclusion in the design and design points with a small prediction variance for deletion from the design. This possibility was omitted in the schematic overview of the algorithm because it provides no additional insights. In order to further speed up the algorithm, powerful routines were used to update the starting design and to evaluate the effect of the design changes in steps 5 and 8. The basic formulae for updating the determinant and the inverse of a nonsingular matrix $\mathbf{A}$ after addition or subtraction of an outer product are given by

$$|\mathbf{A} \pm \mathbf{u}\mathbf{u}'| = |\mathbf{A}|(1 \pm \mathbf{u}'\mathbf{A}^{-1}\mathbf{u})$$

and

$$(\mathbf{A} \pm \mathbf{u}\mathbf{u}')^{-1} = \mathbf{A}^{-1} \mp \frac{(\mathbf{A}^{-1}\mathbf{u})(\mathbf{A}^{-1}\mathbf{u})'}{1 \pm \mathbf{u}'\mathbf{A}^{-1}\mathbf{u}}.$$

Since each design change considered in the algorithm modifies the information matrix of the experiment by adding and subtracting outer products, the determinant and the inverse of the information matrix can be updated by repeatedly using these basic formulae.

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